Simulation Of Planar Heterojunction Solar Cell and Experimental Characterization of Perovskite Materials

SHORT SYNOPSIS

Submitted in partial fulfillment of the requirement of the degree of

DOCTOR OF PHILOSOPHY

by

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ABSTRACT

The aim of the thesis is to fabricate and characterize both theoretically and experimentally perovskite solar cell materials focusing on improving the PCE and stability of the perovskite layer. We have performed two simulation studies to study and observe the various parameters that play a key role in improving the feasibility of the solar cell. The study on the effect of total defect density variation in absorbing layer on the PCE of lead halide perovskite solar cell using SCAPS-1D software has been carried out on the structure ITO/NiO/$CH_3NH_3PbI_3$/SnO_2/Metal resulted in a PCE of 25.5% at the total defect density of $10^{15}cm^{-3}$. We reported another study where the thickness of Nickel Oxide (NiO) or the Hole transport layer was varied. The highest PCE of 53.76% was reported at the layer thickness of 440nm. These numerical observations clearly prove that the perovskite solar cells have the potential to replace the Silicon solar cells in near future.

So, through this work we will try to investigate various bottlenecks in these cells and fabricate a prototype device as a part of experimental work in the laboratory. The proposed device structure will be a layer-by-layer model which will be fabricated using spin coating technique. The device will then be characterized and efficiency will be calculated. The stability of the perovskite layer will be improved using the various other encapsulation techniques. Maximizing efficiency and stability will be the goal of the thesis along with finding a suitable material that can yield much more pronounced results.

Key words: PCE, SCAPS-1D, total defect density, stability, prototype

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1. Introduction

1.1 Overview:

After the crystalline Silicon solar cells much of the emphasis has been laid towards the rapid development of perovskite solar cells. The metal organic-inorganic halide solar cells or lead halide perovskite solar cells are one of the most popular solar cells and have the capability to be commercialized. Till now their reported PCE of 25%. The Power conversion efficiency of such cells can further be improved through the use of various low-cost materials. But these cells suffer a major drawback as lead is considered to be highly toxic that can deplete the environment along with soil and water. So, its use in photovoltaic devices is not a good option. Hence the researchers have shifted their interest towards the use of lead-free perovskite solar cells. Various fabrication techniques have been reported in the literature but still it is a topic of in-depth research. Cesium and Tin are found to be new replacements for lead as these are non-toxic. But still new materials need to be explored. It has been reported that these perovskite cells suffer from degradation due to humidity and various environmental factors. Hence the stability and efficiency of these cells gets affected. Much attention is needed on this subject to improve the overall performance of these devices. Prolonged exposure of the fabricated devices under variation of humidity, temperature etc. is to be done so as to conduct the stability studies [1]. Numerical simulation studies on SCAPS software also showed that these devices have a much wider scope if the layers are optimized in a way that the efficiency gets improved [2].

1.2 Emergence of Lead Halide Perovskites

Photovoltaic technology has gained immense popularity after the advent of Lead Halide based perovskites. Silicon PV technologies have shown an improvement in PCE exceeding 26% and have captured the market. The most established ones are the Si, GaAs and CdTe cells. It has been reported that in past few years lead halide perovskites have surpassed 22% efficiency which is near to CdTe cells. The reported studies conducted by various groups have led to the understanding of the recent developments [3].

1.3 Device structure and configurations

These solar devices have a ABX_3 configuration where A is organic methylammonium or formamidinium (FA) and B site is occupied by lead and X is halogen namely iodine and bromine etc. As far as the structure is considered a TCO or transparent conducting glass is a substrate while the electron selective layer (n-i-p) or hole selective layer (p-i-n) are deposited onto it followed by absorber layer and topped electron and hole layer and the metal contact.

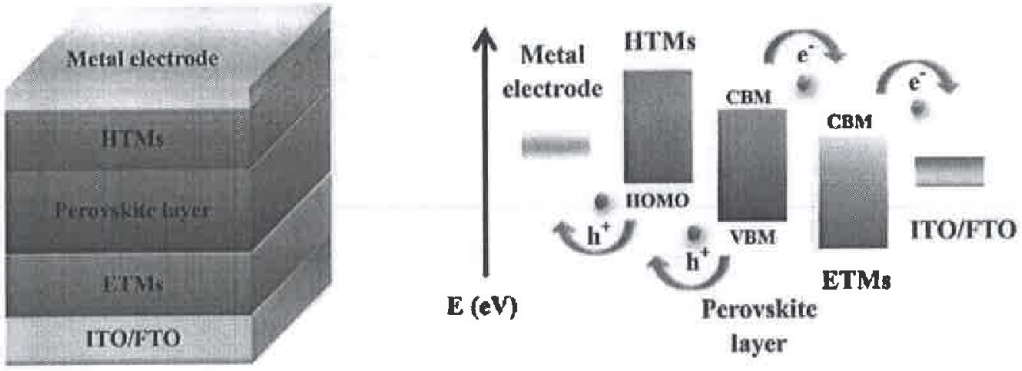

Figure1: (a) Schematic diagram of perovskite solar cell. (b) Working principle of perovskite solar cell [4]

1.4 Lead-free perovskite solar cells

As the lead- based perovskite solar cells are toxic, they pose a danger to the environment and that is why they have been failed to commercialize although they have enormous potential. If lead is being replaced by a non-toxic material, then its toxicity can be reduced to a larger extent for solar cell fabrication. One of the research groups have published simulation studies using SCAPS software on Cs_2TiBr_6 compound that forms an absorber layer. The efficiency of this cell has been reported to be about 17.83%. the device structure is Au/PEDOT: PSS/Cs_2TiBr_6/TiO_2/AZO. For designing the solar cells, we need to first concentrate on the absorber layer as this layer is responsible for absorbing photons and the balanced movement of charges inside the solar cell is responsible for the maximum generation of power. The absorbing layer or the perovskite layer is the prime focus of research [5].

1.5 Challenges with perovskite solar cells

These cells suffer degradation after a certain period of time and thus their overall performance gets affected which leads to poor efficiency and deteriorated stability. Prolonged exposure to

moisture and various other environmental factors causes complete failure of the device. So, this is the main reason that these cells have failed to take over the market.

2. Literature Review

(Correa-Baena et al., n.d.) presented the advancement of perovskite solar cells and their potential to replace the Si, CdTe and GaAs solar cells. It talks about the lead halide perovskites that can replace the above solar cells. They have shown a efficiency of 26%. The group has highlighted long term stability issue that these cells suffer from and that is why they have not been able to commercialize. Apart from this they have talked about various extrinsic and intrinsic factors responsible for the degradation of these cells [6].

(Meng et al., 2018) reported the key metrics that are required to translate photovoltaic technology from laboratory to the market. These metrics are low-cost, high-power conversion efficiency and high stability. The organic-inorganic metal halides remain practically irrelevant due to their low operation time. The longest lifetime reported is 1 year for such cells which is 25 years for the commercialized PV cells. So much attention has to be laid in order to achieve high stability. Encapsulation has to be done so as to prevent these cells from humidity and moisture. The three main intrinsic factors responsible for instability are ion migration, hygroscopicity and thermal instability. Thermal instability can be resolved by composition tuning, hygroscopicity by encapsulation and ion migration by A site alkali doping and replacement [7].

Table 1: Comparative study of various methods for perovskite layer fabrication [8]

S.No.	Method	Roll to Roll	Pattern	Single cell efficiency
1	Blade coating	yes	No	19.5
2	Slot-die coating	yes	yes	14.7
3	Spray coating	yes	yes	18.3
4	Inkjet printing	yes	yes	12.3
5	Screen printing	yes	yes	15.6

(Li et al., 2018) have reported various methods to fabricate scalable roll to roll perovskite solar cells and have drawn the comparisons also. The various methods have been tabulated above.

In this research article **(Dehghanipour et al., 2021)** have reported the post treatment process that is given to Perovskite solar cells in order to increase their stability. In this study Tetrabutylammonium Tetrafluoroborate ($TBABF_4$) is used as a passivator to improve the performance of the fabricated PSCs. Through the treatment using above solvent the film's grain boundaries were passivated which reduces the charge traps on the surface of the perovskite layer. To further investigate the effect of this solvent after post treatment on the optical properties and charge recombination process photoluminescence measurements were done at wavelength of 405nm. It was found that the PL spectra was consistent with the previous reports as it showed a PL peak around 800nm with a bandgap of 1.55eV [9].

The group led by **(Chandra & Mandal, 2022)** [10] explained the morphology control in $(CH_3NH_3)_3Bi_2Cl_9$ thin film for lead free perovskite solar cells. Traditional perovskites have shown remarkable progress but presence of toxic lead have hindered their commercialization. So, the group reported MABiCl thin perovskite based solar cell. Their process showed uniform morphology of film, high open circuit voltage and good fill factor. An open circuit voltage of 496mV and FF of 0.55 was measured. The reduced traps on the surface decreased the possibility of recombination of photoexcited charge carriers **(Meng et al., 2018)** [7] also reported that toxicity of lead is a major drawback that diminishes stability of the PSCs. Additionally **(Chandra & Mandal, 2022)** [10] have reported the fabrication process of this light absorber solar cell material. They have mixed CH_3NH_3Cl in DMF in a given ratio and then stirred it 50°C for half an hour followed by addition of ethyl alcohol and vacuum drying.

The group led by **(Jain et al., 2019)**explained the use of P3HT and Spiro-OMeTAD as the HTL (Hole transport materials) that yielded the efficiency of 1.12 and 1.62% respectively. They have synthesized high quality films using methyl acetate as the solvent. The quality of films was confirmed from XRD, X-Ray photoelectron spectroscopy etc [11].

A theoretical investigation on the effect of hole and electron transport materials on the on the performance of lead-free PSC based on $CH_3NH_3SnI_3$ has been reported by **(Rono et al., 2021).** The simulation studies were done on SCAPS-1D simulator software. The structure simulated was glass/FTO/WS2/ $CH_3NH_3SnI_3$ /P3HT/Au and it showed a PCE of 10.47%. They have tested various ETL and HTL materials and reported their efficiencies. They have stated that changing the HTL to CU_2O and ETL to WS_2 remarkedly increased the efficiency to 16.40% [12].

(Mahajan et al., 2021) have talked about the advances that are made in the field of tin-based perovskite solar cells. They have summarized the developments that are made in this area since 2014. They have reviewed $MASnI_3$, $FASnI_3$, $CsSnI_3$ and mixed cation tin perovskites. These have known to reach a PCE of 9.6%. $MASnI_3$ have achieved an efficiency of 7.78% with high stability and reproducibility. $FASnI_3$ reached efficiency of 12.4% using ICBA as ETL. The maximum attainable voltage is 0.94V. ICBA incorporated solar cell maintained 90% of its original efficiency for 3800 hours. For $CsSnI_3$ films solvothermal process was used and they attained 12.96% efficiency. After all such experiments the group concluded that the stability of Tin based perovskites much poorer than Lead based perovskites. So, in near future efforts should be made to improve their stability [13].

Another numerical study is done by a group **(Gamal et al., 2021)** using SCAPS-1D simulator in which ZnMgO is taken as the ETL and $CH_3NH_3SnI_3$ is taken as absorber layer. Different HTL materials were taken to find the best suitable. MASnBr3 taken as HTL provided the open circuit voltage Voc as 0.95V, FF of 82.01 and PCE of 26.33%. The purpose of conducting this research is to design and improve the efficiency lead-free PSC due to problem of low absorption in UV range. This problem can be overcome by ZnMgO as it has a wider energy band gap. They have mentioned that the thickness of absorber layer must be optimized in a way that it should not be too thick or too thin. This study has provided a guideline to design such cells in the future [14].

Ion migration process that affects the stability of perovskite solar cells is being reviewed by **(Zhao et al., 2021)** in this study. This is the main cause of degradation of such solar cells.

Characterization methods such as ion impedance have been reviewed. They have provided several solutions to mitigate this but these are not enough to commercialize them as some methods are too expensive while other use highly toxic solvents that will ruin the environment. They have suggested that while preparing the ETL layer the nanoparticles must be dispersed in water while doing the spin coating. Thermal stability should also be considered. HTL layer should be modified so that its interface with absorber layer is not disturbed. But much more experimentation is needed [15].

3. Description of Broad Area

The broad topic of research is perovskite solar cells. These cells have a potential to replace the silicon solar cells but their stability issues are a major hindrance towards their commercialization. Improving the performance of the lead halide perovskite solar cells is the main aim of the work. Lead-free perovskites are a class of perovskite solar cells in which the absorber layer will be free from lead. The proposed structure of the device will be formulated and experimental as well as simulation studies will be performed on the structure. Then various characterizations will be done and efficiency will be determined. A comparison between the theoretical and experimental values will be drawn.

4. Objectives of the study

1) To simulate the perovskite based solar cell structure by SCAPS-1D software and calculate the various cell parameters.

2) The proposed research aims to synthesize perovskite materials in laboratory and characterize them.

3) To characterize various synthesized perovskite materials for solar cell.

5. Methodology

The thesis will comprise both of theoretical and experimental work.

- **Theoretical work**: The simulation studies will be carried out on SCAPS software. The proposed structure will be simulated and the efficiency will be calculated.
- **Experimental work**: The prototype device will be fabricated in the laboratory using spin coating technique. All the layers will be optimized first and then the device will be fabricated.The nanocomposite thin films of desired thickness will be deposited on the ITO /FTO substrate. After this the characterization of the device will be performed and efficiency will be calculated.

6. Expected outcome of research

We will try to fabricate a prototype device to the best of our efforts that will have an improved power conversion efficiency and stability.

- Standard development
- Efficiency improvement
- Stability improvement
- Cost reduction

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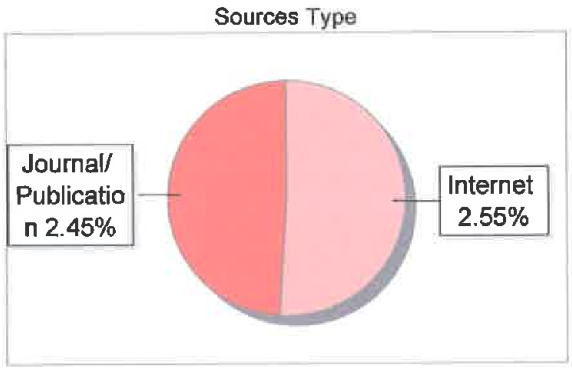

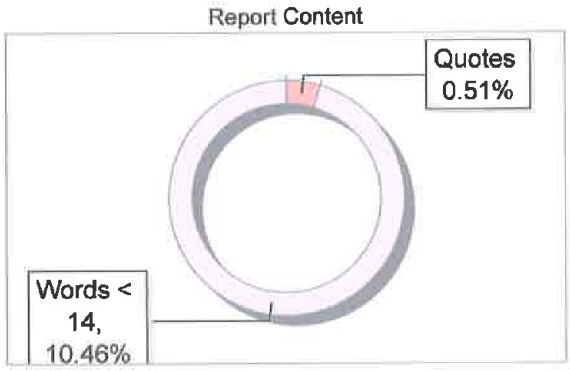

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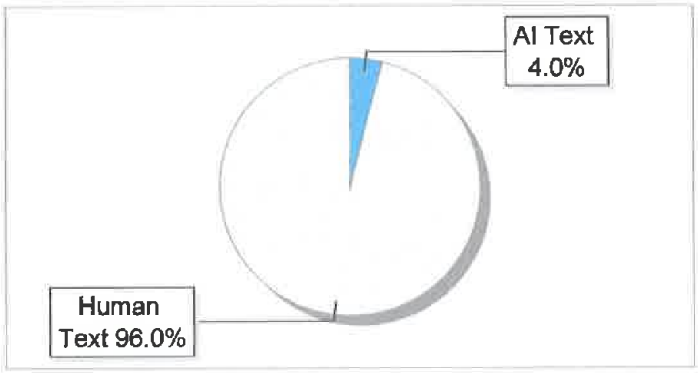

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